Optimized and Quasi-Optimal Schwarz Waveform Relaxation for the One Dimensional Schrödinger equation

Laurence Halpern[1] and Jérémie Szeftel[2]

[1] LAGA UMR 7539

Université Paris 13

[2] Department of Mathematics

Princeton University

and

MAB UMR 5466

Université Bordeaux 1

The Schrödinger equation

$$\begin{cases} i\partial_t u(t,x) + \partial_x^2 u(t,x) + V(x)u(t,x) = 0 \\ u(0,x) = u_0(x) \end{cases}$$

Quantum mechanics, electromagnetic wave propagation,

optic (Fresnel equation)

Goal : Design efficient Schwarz Waveform Relaxation algorithms

for the Schrödinger equation

Schwarz Waveform Relaxation algorithm

= global in time domain decomposition method

Classical Schwarz Waveform Relaxation

Optimal Schwarz Waveform Relaxation Algorithm

The Quasi-Optimal Algorithm

The Robin Algorithm

Numerical schemes

Numerical results

Classical Schwarz Waveform Relaxation

$$\begin{cases} (i\partial_t + \partial_x^2 + V)u_1^k = 0 \text{ in } \Omega_1 \times (0,T) \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1 \\ u_1^k(L,\cdot) = u_2^{k-1}(L,\cdot) \text{ in } (0,T) \end{cases} \qquad \begin{cases} (i\partial_t + \partial_x^2 + V)u_2^k = 0 \text{ in } \Omega_2 \times (0,T) \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2 \\ u_2^k(0,\cdot) = u_1^{k-1}(0,\cdot) \text{ in } (0,T) \end{cases}$$

Convergence factor :

$$\Theta(\tau,L) = exp\left[-\left(\frac{-\tau+V+\sqrt{1+(\tau-V)^2}}{2}\right)^{1/2} L\right]$$

$$\lim_{\tau\to+\infty} \Theta(\tau,L) = 1$$

Movie : slow convergence of the Classical Schwarz Waveform Relaxation

Free Schrödinger equation

Computation over $\Omega_1 = (-5, 4\Delta x)$ and $\Omega_2 = (0, 5)$ for $0 \leq t \leq 0.5$

$\Delta t = 0.00125$, $\Delta x = 0.0125$

Movie : absolute value of the exact solution (—) and of the solution computed with the Classical Schwarz algorithm (—)

200 iterations

Optimal Schwarz Waveform Relaxation Algorithm

$$\begin{cases} (i\partial_t + \partial_x^2 + V)u_1^k = 0 \text{ in } \Omega_1 \times (0,T) \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1 \\ (\partial_x + \mathcal{S}_1)u_1^k(L,\cdot) \\ = (\partial_x + \mathcal{S}_1)u_2^{k-1}(L,\cdot) \text{ in } (0,T) \end{cases} \quad \begin{cases} (i\partial_t + \partial_x^2 + V)u_2^k = 0 \text{ in } \Omega_2 \times (0,T) \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2 \\ (\partial_x + \mathcal{S}_2)u_2^k(0,\cdot) \\ = (\partial_x + \mathcal{S}_2)u_1^{k-1}(0,\cdot) \text{ in } (0,T) \end{cases}$$

Convergence in 2 iterations if and only if

$$\sigma_1 = (\tau - V)^{1/2}, \quad \sigma_2 = -(\tau - V)^{1/2}$$

$$(\tau - V)^{1/2} = \begin{cases} \sqrt{\tau - V} \text{ if } \tau \geq V \\ -i\sqrt{-\tau + V} \text{ if } \tau < V \end{cases}$$

For non constant V : optimal operators not at hand

The Quasi-Optimal Algorithm

$$\begin{cases} (i\partial_t + \partial_x^2 + V)u_1^k = 0 \text{ in } \Omega_1 \times (0,T) \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1 \\ (\partial_x + \sqrt{-i\partial_t - V(L)})u_1^k(L,\cdot) \\ = (\partial_x + \sqrt{-i\partial_t - V(L)})u_2^{k-1}(L,\cdot) \end{cases} \quad \begin{cases} (i\partial_t + \partial_x^2 + V)u_2^k = 0 \text{ in } \Omega_2 \times (0,T) \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2 \\ (\partial_x - \sqrt{-i\partial_t - V(0)})u_2^k(0,\cdot) \\ = (\partial_x - \sqrt{-i\partial_t - V(0)})u_1^{k-1}(0,\cdot) \end{cases}$$

$$(\tau - V(x))^{1/2} = \begin{cases} \sqrt{\tau - V(x)} \text{ if } \tau \geq V(x) \\ -i\sqrt{-\tau + V(x)} \text{ if } \tau < V(x) \end{cases}$$

The algorithm converges in

$$(H^{1/4}(0,T,L^2(\Omega_1)) \cap H^{-1/4}(0,T,H^1(\Omega_1))) \times (H^{1/4}(0,T,L^2(\Omega_2)) \cap H^{-1/4}(0,T,H^1(\Omega_2)))$$

The Robin Algorithm

Zero order approximation of the Optimal Algorithm :

$$\begin{cases} (i\partial_t + \partial_x^2 + V)u_1^k = 0 \text{ in } \Omega_1 \times (0,T) \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1 \\ (\partial_x - ip)u_1^k(L,\cdot) \\ = (\partial_x - ip)u_2^{k-1}(L,\cdot) \text{ in } (0,T) \end{cases} \begin{cases} (i\partial_t + \partial_x^2 + V)u_2^k = 0 \text{ in } \Omega_2 \times (0,T) \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2 \\ (\partial_x + ip)u_2^k(0,\cdot) \\ = (\partial_x + ip)u_1^{k-1}(0,\cdot) \text{ in } (0,T) \end{cases}$$

Complex Robin algorithm

For any $p > 0$, the algorithm converges in

$$L^\infty(0,T;L^2(\Omega_1)) \times L^\infty(0,T;L^2(\Omega_2))$$

Optimization with respect to $p > 0$ to improve the convergence

Numerical schemes

Finite volumes discretization

Interior = Crank Nicolson scheme

Quasi-Optimal algorithm : discretize $\sqrt{-i\partial_t + V}$

Approximation of Arnold and Ehrhardt

$$\sqrt{-i\partial_t + V}U(0,n) \simeq \sum_{m=0}^{n} S(n-m)U(0,m)$$

where $S(m)$ is given by a recurrence formula

Other possible approximations : Lubich and Schädle,

Schmidt and Yevick, Antoine and Besse, ...

Numerical results

Optimal p for the Robin algorithm

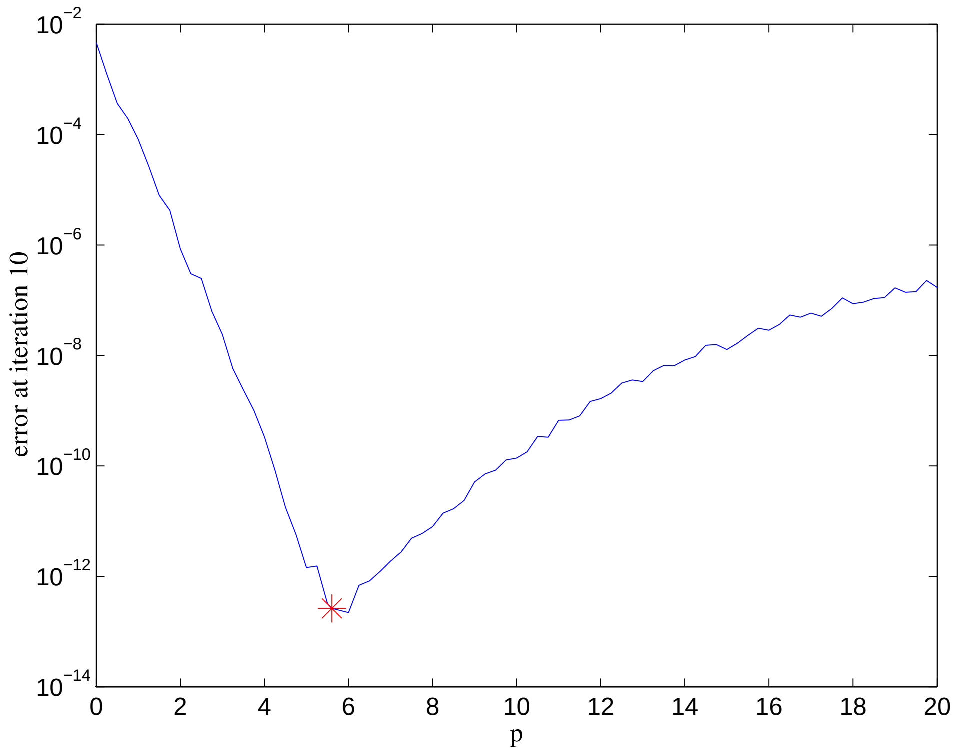

FIG. 1 – Variation of the quadratic error in time and space in Ω_1 as a function of p. The overlap is equal to 1%. The star corresponds to the theoretical optimal value p_T. Free Schrödinger equation

Comparison Classical/Robin algorithms

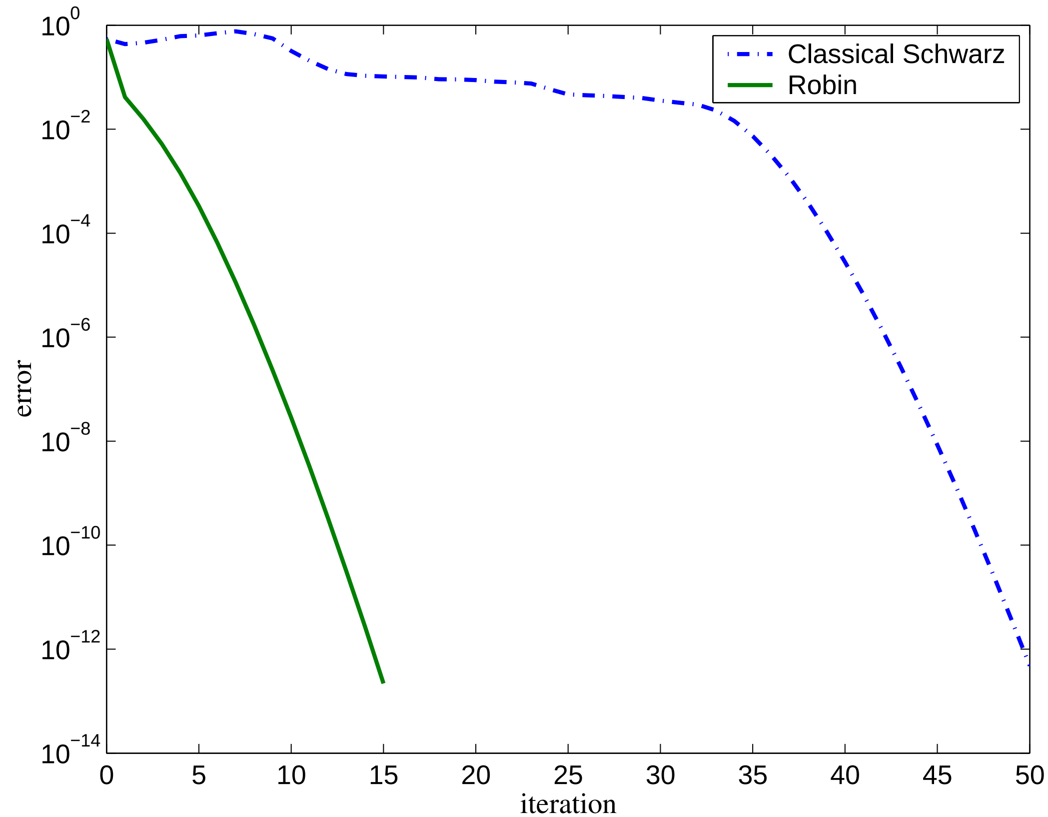

FIG. 2 – Convergence history : comparison of the Classical and Optimized Robin Schwarz algorithm. Free Schrödinger equation. $\delta = 2\%$

Robin algorithm without overlap

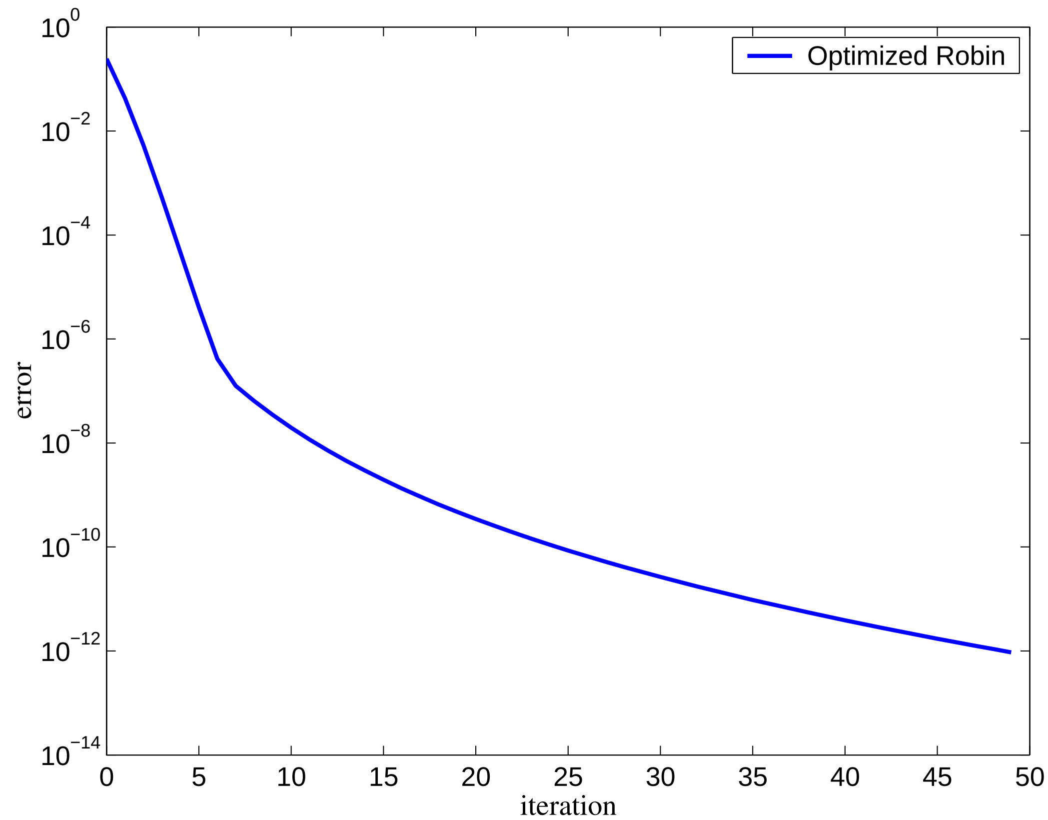

FIG. 3 – Convergence history for the Optimized Robin Schwarz algorithm in the non overlapping case. Free Schrödinger equation

Comparison Classical/Robin algorithms

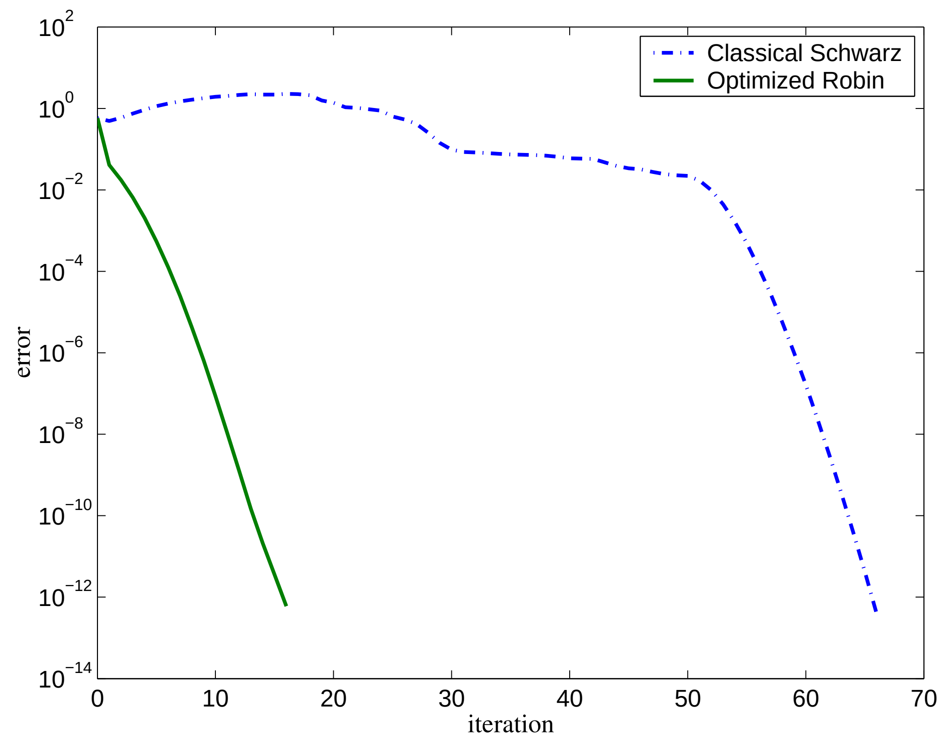

Fig. 4 – Convergence history : comparison of the Classical and Optimized Robin Schwarz algorithm for a potential barrier. The overlap is equal to 4%

The Quasi-Optimal algorithm

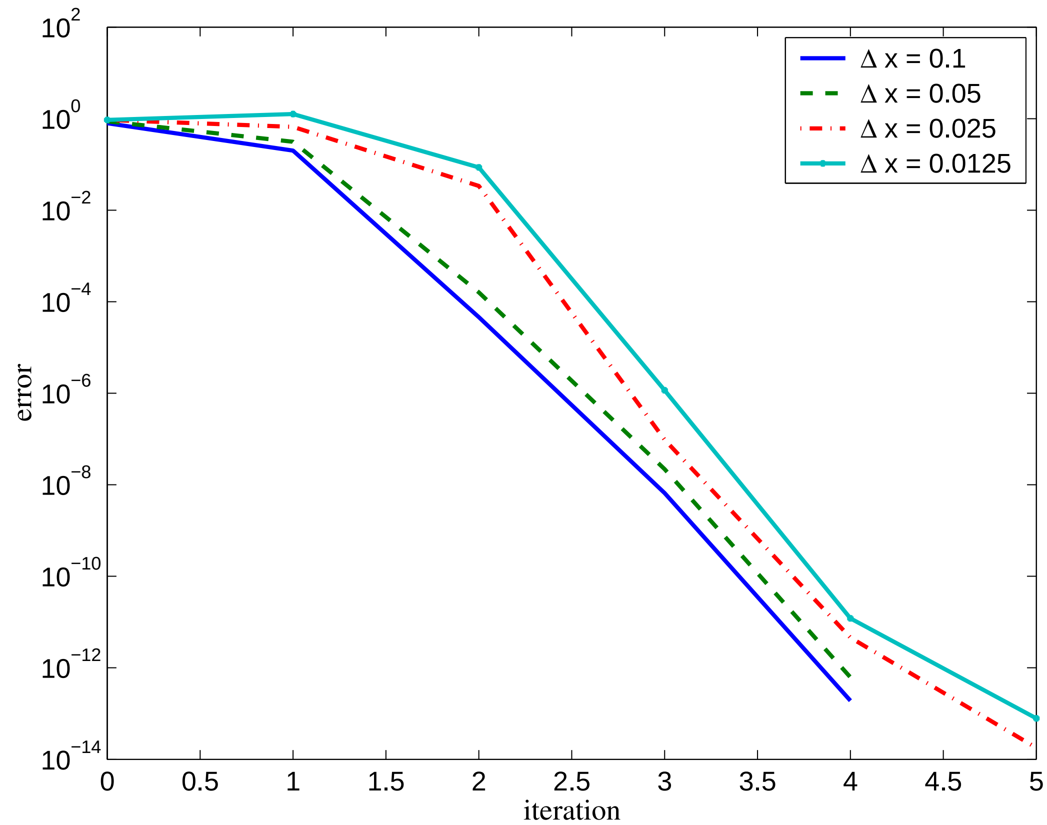

FIG. 5 – Convergence history for the Quasi-Optimal Schwarz algorithm in presence of a parabolic potential

Movie : Comparison of the Classical, Robin and Quasi-Optimal algorithms

The Schrödinger equation with a parabolic potential

Computation over $\Omega_1 = (-5, 4\Delta x)$ and $\Omega_2 = (0, 5)$ for $0 \leq t \leq 1$

$\Delta t = 0.0025$, $\Delta x = 0.025$

Movie 1 : absolute value of the exact solution (—) and of the solution computed with the Classical Schwarz algorithm (—)

Movie 2 : absolute value of the exact solution (—) and of the solution computed with the Robin algorithm (—)

Movie 3 : absolute value of the exact solution (—) and of the solution computed with the Quasi-Optimal algorithm (—)

3 iterations

Conclusions and perspectives

- The Classical algorithm converges extremely slowly for the Schrödinger equation with or without a potential
- We have designed two alternative algorithms : a Complex Optimized Robin algorithm and a Quasi-Optimal algorithm
- These algorithms greatly improve the performances of the classical Schwarz relaxation algorithm
- We intend to extend our analysis to the two-dimensional case in a close future